SYSTEM AND METHOD FOR SCANNING NEAR-FIELD
OPTICAL TOMOGRAPHY

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BACKGROUND OF THE INVENTION

1. Field of the Invention

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This invention relates to tomography and, more particularly, to near-field microscopy wherein an image of an object is directly reconstructed with sub-wavelength resolution.

15   2. Description of the Background Art

Near-field scanning optical microscopy (NSOM) is a technique to obtain images of surfaces with sub-wavelength resolution. The technique is particularly important for imaging structures where spectroscopic concerns or sample handling 20 requirements dictate the use of lower frequency fields and yet high spatial resolution is still required. Applications range from the inspection of organic and biological samples to semiconductors. Various modalities are in practical use. Two prominent examples of such modalities are "illumination mode NSOM" and "collection mode NSOM". In illumination mode NSOM, a tapered fiber probe with a sub-wavelength size aperture 25 serves as a source of illumination in the near-zone of the sample. The scattered field intensity is then measured and recorded as a function of the probe position while the probe is scanned over the sample. In collection mode NSOM, the fiber probe serves to detect the scattered field in the near-zone as the sample is illuminated by a source in the far zone.

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There are certain limitations of current NSOM techniques. Despite the fact that the sample may present a complicated three-dimensional structure, NSOM produces only a two-dimensional image of the sample. Indeed, rather than being an imaging method, it is more accurate to say that NSOM maps the sub-wavelength

5   structure of the optical near-field intensity. Under certain simplifying assumptions, such as homogeneity of the bulk optical properties of the sample, the maps produced in these experiments may be related to the sample structure. However, for the more general case in which the topography of the sample and the bulk optical properties both vary, the connection between the near-field intensity and the sample structure can be ambiguous.

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To resolve this ambiguity it is desirable to solve the inverse scattering problem (ISP). The ISP may be characterized as reconstructing the three-dimensional object structure, in this case the dielectric susceptibility of the sample, from measurements of the scattered field. By solving the ISP, two main issues of the prior art

15   are resolved, namely, the ambiguity in connecting the sample properties and the measured data is resolved, and simultaneously three-dimensional, tomographic images of the sample are obtained.

Historically, solving the ISP for other scattering modalities has greatly

20   expanded the functionality of existing methods. For instance, pioneering analysis of X-ray diffraction made modern crystallography a reality. Another pioneering work brought medical imaging out of the era of projection radiography and into the era of computed tomography (CT). In any ISP the first step is to obtain a physically reasonable forward

model for the scattering process. For instance, in CT, a geometric model of propagation, neglecting any scattering, sufficiently describes the experiment. Likewise, as scattering becomes important, the first Born approximation is a reasonable model. By considering the far-zone scattered field, one may obtain a readily soluble ISP, now generally known

5   as diffraction tomography (DT). The crucial step in the DT solution is to obtain a linearized relationship between the sample properties and the scattered field or some simple function of the scattered field. This may be accomplished by making use of models such as the first Born or first Rytov approximations. Solutions for the non-linear ISP may be obtained as well, but in general they suffer from mathematical

10   pathologies involving convergence.

        The far-zone ISP has an inherent resolution limit imposed by the wavelength of the probe field. This limit may be traced to the fact that only the homogeneous part of the scattered field contributes to the far-zone. While in principle a

15   higher resolution image may be obtained by mathematical extrapolation, this approach is exponentially sensitive to errors in the scattering data. However, the evanescent waves which contribute to the near-field carry the higher spatial frequency information about the scatterer. It is known that inclusion of the evanescent waves in the standard back propagation algorithm of two-dimensional DT enhances the resolving power of that

20   method.

        The sub-wavelength resolution obtained in NSOM arises because direct access to the evanescent scattered waves by probing the near-field is effected. It is this

part of the scattered field on which the sub-wavelength structure of the scattering object is encoded. The NSOM ISP is thus of great interest because it obtains sub-wavelength resolved three-dimensional reconstructions. This technique, in accordance with the present invention, is referred to this as "scanning near-field optical tomography".

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Representative of the art in this technological area are the following U.S. Patents: (a) Fiber Optic Probe for Near Field Optical Microscopy (No. 5,485,536); (b) Method and Apparatus for Performing Near-Field Optical Microscopy (No. 5,479,024); (c) Near Field Scanning Tunneling Optical Microscope (No. 5,382,789; and (d) Near

10   Field Optical Microscopic Examination of a Biological Specimen (No. 5,286,970).

The art is devoid of any teachings or suggestions for treating the inverse scattering problem which is applicable to the near-field case.

15   SUMMARY OF THE INVENTION

These shortcomings, as well as other limitations and deficiencies are obviated, in accordance with the present invention, by devising explicit inversion formulas that are applicable to near-field scanning optical tomography and which provide a direct reconstruction of a scattering potential associated with a sample being scanned.

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In accordance with a broad method aspect of the present invention related to scalar waves, an image of an object is generated by: (a) probing the object with incident scalar waves; (b) detecting scattered waves from the object, wherein the

scattered waves are detected in a near-field collection mode; and (c) reconstructing the tomographic image by executing a prescribed mathematical algorithm with reference to the incident scalar waves and the scattered waves to generate the tomographic image with sub-wavelength spatial resolution.

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In accordance with another broad method aspect of the present invention related to scalar waves, an image of an object is generated by: (a) probing the object with incident scalar waves, wherein the incident scalar waves are generated in a near-field illumination mode; (b) detecting scattered waves from the object, wherein the scattered

10　　waves are detected in the far-field of the object; and (c) reconstructing the tomographic image by executing a prescribed mathematical algorithm with reference to the incident scalar waves and the scattered waves to generate the tomographic image with sub-wavelength spatial resolution.

15　　In accordance with yet another broad method aspect of the present invention related to scalar waves, an image of an object is generated by: (a)　probing the object with incident scalar waves, wherein the incident scalar waves are generated in a near-field illumination mode; (b) detecting scattered waves from the object, wherein the scattered waves are detected in a near-field collection mode; and (c) reconstructing the

20　　tomographic image by executing a prescribed mathematical algorithm with reference to the incident scalar waves and the scattered waves to generate the image with sub-wavelength spatial resolution.

In accordance with a broad method aspect of the present invention related to electromagnetic waves, an image of an object is generated by: (a) probing the object with incident electromagnetic waves; (b) detecting scattered waves from the object, wherein the scattered waves are detected in a near-field collection mode; and (c)

5   reconstructing the tomographic image by executing a prescribed mathematical algorithm with reference to the incident electromagnetic waves and the scattered waves to generate the tomographic image with sub-wavelength spatial resolution.

In accordance with another broad method aspect of the present invention

10   related to electromagnetic waves, an image of an object is generated by: (a) probing the object with incident electromagnetic waves, wherein the incident electromagnetic waves are generated in a near-field illumination mode; (b) detecting scattered waves from the object, wherein the scattered waves are detected in the far-field of the object; and (c) reconstructing the tomographic image by executing a prescribed mathematical algorithm

15   with reference to the incident electromagnetic waves and the scattered waves to generate the tomographic image with sub-wavelength spatial resolution.

In accordance with yet another broad method aspect of the present invention related to electromagnetic waves, an image of an object is generated by: (a)

20   probing the object with incident electromagnetic waves, wherein the incident electromagnetic waves are generated in a near-field illumination mode; (b) detecting scattered waves from the object, wherein the scattered waves are detected in a near-field collection mode; and (c) reconstructing the tomographic image by executing a prescribed

mathematical algorithm with reference to the incident electromagnetic waves and the

scattered waves to generate the image with sub-wavelength spatial resolution.

Broad system aspects of the present invention are commensurate with

5   these method aspects.

BRIEF DESCRIPITON OF THE DRAWING

FIG. 1 is a pictorial representation for the single probe illumination mode

10   showing an object under test;

FIG. 2 is a pictorial representation for the single probe collection mode showing

an object under test;

FIG. 3 is a pictorial representation for the two-probe mode showing an object

under test;

15   FIG. 4 depicts a system for probing the object with waves to produce scattered

waves which are then used to directly reconstruct the image; and

FIG. 5 is a flow diagram for directly reconstructing the image of the object

excited by a probing wave.

DETAILED DESCRIPTION

1. OVERVIEW

5   When both the phase and amplitude of the optical near-field are

measurable, the near-field ISP may be solved, and robust inversion algorithms for both

the scalar and vector near-field scattered waves may be obtained.   In this detailed

description, three example modalities are treated. The treatment of the vector case is

particularly important in the near-field ISP because polarization effects are somewhat

10   more complicated than for the far-field problem.   The solution in all cases is derived by a

singular value decomposition (SVD) analysis of the linearized scattering problem. The

SVD is a generalized mode decomposition that offers considerable insight into the

scattering problem.

15   In Section 2, a discussion of near-field scattering for scalar wave-fields

obeying the scalar reduced wave equation is presented. Specifically, expressions for the

scattered field as measured in three distinct modalities are obtained. The first two

modalities are variations on the illumination mode and collection mode techniques. It is

presumed that the field may be measured, that is, the measurements are phase sensitive.

20   Moreover, the third modality requires the use of two near-field probes. The three

expressions derived for the scattered fields are shown to be special cases of a single

expression relating the measured data to the structure of the scattering object to be

imaged.

In Section 3, a unified form for all three modalities is treated and it is shown that, in all cases, a unique solution of the inverse scattering problem exists. Furthermore, the SVD for the scattering kernel is then developed and the inversion formula for the ISP is obtained.

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In Section 4 the vector theory of near-field scattering is presented. The three modalities are again discussed, as well as the unified form of the modalities.

In Section 5, the existence and uniqueness of the solution to the inverse

10   scattering problem is demonstrated and the SVD is developed. It will be seen that though the vector nature of light makes a significant difference in the physics of the problem, the underlying mathematical form is much like the scalar case and the results follow from the scalar case in a straight-forward manner.

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2. FUNCTION THEORETIC BASIS FOR SCALAR SCATTERING

To understand the principles in accordance with the present invention, the case wherein a monochromatic scalar plane wave of frequency ω incident on a medium

20   characterized by a scattering potential $\eta(r)$ is first considered. The field $U(r)$ of the wave satisfies the reduced wave equation

$$\nabla^2 U(r) + k_0^2 U(r) \; = \; -4\pi k_0^2 \eta(r) U(r) \tag{1}$$

where $k_o^2 = 2\pi / \lambda = \omega/c$ is the free-space wavenumber of the incident wave. The field is then composed of two parts, namely,

$$U(\mathbf{r}) = U_i(\mathbf{r}) + U_s(\mathbf{r}), \tag{2}$$

with the incident field $U_i(\mathbf{r})$ satisfying the free-space reduced wave equation,

$$\nabla^2 U_i(\mathbf{r}) + k_0^2 U_i(\mathbf{r}) = 0, \tag{3}$$

and the scattered field $U_s(\mathbf{r})$ satisfying the equation

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$$\nabla^2 U_s(\mathbf{r}) + k_0^2 U_s(\mathbf{r}) = -4\pi k_0^2 \eta(\mathbf{r}) U(\mathbf{r}). \tag{4}$$

Following standard procedures, equation (4) may be recast as the integral equation

$$U_s(\mathbf{r}) = k_o^2 \int d^3 r' G(\mathbf{r} - \mathbf{r}') \eta(\mathbf{r}') U(\mathbf{r}'), \tag{5}$$

where

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$$G(\mathbf{r} - \mathbf{r}') = \frac{1}{4\pi} \frac{e^{ik_0|\mathbf{r} - \mathbf{r}'|}}{|\mathbf{r} - \mathbf{r}'|} \tag{6}$$

is the outgoing-wave Green's function for equation (4) which obeys

$$\nabla^2 G(\mathbf{r}) + k_0^2 G(\mathbf{r}) = -4\pi\delta(\mathbf{r}). \tag{7}$$

If the scattered field is much weaker than the incident wave, the first Born approximation

15   applies and the following is obtained from equation (5):

$$U_s(\mathbf{r}) = k_o^2 \int d^3 r' G(\mathbf{r} - \mathbf{r}') \eta(\mathbf{r}') U_i(\mathbf{r}'). \tag{8}$$

In the discussion that follows, it will prove useful to express the Green's function G in

the plane wave decomposition

$$G(\mathbf{r}) \;=\; \frac{i}{2\pi} \int d^2 Q \, k_z(Q)^{-1} \exp[iQ \cdot \rho + i k_z(Q)\,|z\,|], \tag{9}$$

where $k_z(Q) = (k_0^2 - Q)^{\frac{1}{2}}$. The modes appearing in equation (9) labeled by Q for which $|Q| \le k_0$ are the homogeneous wave modes. The modes labeled by Q for which $|Q| > k_0$ are evanescent. For these modes, $k_z(Q) = i\,|k_z(Q)|$ so that the evanescent waves decay

5   exponentially on propagation, with a concomitant loss of high-spatial frequency

components in the scattered field.

2A. Illumination Mode

Next consider the case in which the sample is illuminated by a point

10   source with unit amplitude at the position r_1 with

$$U_i(\mathbf{r}) = \frac{e^{ik_0|\mathbf{r}-\mathbf{r}_1|}}{|\mathbf{r}-\mathbf{r}_1|}. \tag{10}$$

This arrangement is shown pictorially in FIG. 1 wherein probe **101** is

representative of a source which illuminates sample **105**. The illumination as reflected

15   from sample **105** is depicted by reflected wave **102**, and the illumination as transmitted

by sample **105** is depicted by transmitted wave **103**.

The scattered field at a point r is then given by the expression

$$U_s(\mathbf{r}) = k_0^2 \int d^3 r'\, G(\mathbf{r}-\mathbf{r}')\eta(\mathbf{r}')G(\mathbf{r}'-\mathbf{r}_1). \tag{11}$$

20   It is assumed that the source lies in the plane $z = 0$ so that the position of the source is

$r_1 = (\rho_1,0)$ with ρ_1 being the transverse coordinate of the source. The scatterer is

- 11 -

assumed to lie only in the half-space $z \geq 0$ and to be of finite range. If the scattered field

is measured in the $z > 0$ half-space, this scattered field is referred to as the "transmission

mode". If the scattered field is measured in the $z \leq 0$ half-space, this scattered field is

referred to as the "reflection mode". It is now supposed that the observation point r is

5   very far from the domain of the scatterer. Then observe that for $|r| >> |r'|$

$$G(r - r') \sim \frac{e^{ik_0 r}}{r} e^{-ik(q) \cdot r'} \qquad (12)$$

where $k(q) = (q, \varepsilon k_z(q))$ is parallel to r. Here $\varepsilon = 1$ for the transmission mode, and

$\varepsilon = -1$ for the reflection mode. It is then seen that the scattered field may be expressed in

terms of the scattering amplitude $A(\rho_i, q)$ as

10
$$U_s(r) \sim \frac{e^{ik_0 r}}{r} A(\rho_1, q), \qquad (13)$$

where with the use of equations (9), (11), and (12) it is found that

$$A(\rho_1, q) = k_0^2 \int d^3 r' G(r' - r_1) \exp[-iq \cdot \rho' - i\varepsilon k_z(q) z'] \eta(r'). \qquad (14)$$

Now define a data function $\Phi_1(q_1, q_2)$ by a two-dimensional Fourier

15   transform of $A(\rho_1, q)$,

$$\Phi_1(q_1, q_2) = \frac{1}{2\pi} \int d^2 \rho_1 e^{iq_1 \cdot \rho_1} A(\rho_1, q_2). \qquad (15)$$

Making use of equations (9) and (14), it is readily shown that

$$\Phi_1(q_1, q_2) = \frac{ik_0^2}{k_z(q_1)} \int d^3 r \exp\{i(q_1 - q_2) \cdot \rho + i[k_z(q_1) - \varepsilon k_z(q_2)]z\} \eta(r). \qquad (16)$$

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2B. Collection Mode

In this modality, the sample **105** is illuminated from the far zone by an incident plane wave and the scattered field is detected in the near-zone by means of an idealized point detector. This arrangement is shown pictorially in FIG. 2 wherein probe

5   **201** is representative of a detector which collects scattered waves from sample **105**. Sample **105** is illuminated by incident wave **202** in the reflection mode, whereas sample **105** is illuminated by incident wave **203** in the transmission mode.

The incident wave is taken to have unit amplitude and is of the form

$$U_i(\mathrm{r}) = \exp[iq \cdot \rho - i\varepsilon k_z(q)z], \tag{17}$$

10   where, once again, $\varepsilon = 1$ for the transmission mode and $\varepsilon = -1$ for the reflection mode. The scattered field, measured in the $z = 0$ plane at a point with transverse coordinate ρ, is given by the expression

$$U_s(\rho,0;q) = k_0^2 \int d^3r' \exp[iq \cdot \rho' - i\varepsilon k_z(q)z] G(\mathrm{r}'-\mathrm{r})\eta(\mathrm{r}'), \tag{18}$$

which follows from equation (8). As in the illumination mode case, a data function

15   $\Phi_2(q_1,q_2)$ is defined by a Fourier transform of the scattered field

$$\Phi_2(q_1,q_2) = \frac{1}{2\pi} \int d^2\rho\, e^{-iq_2 \cdot \rho} U_s(\rho,0;q_1). \tag{19}$$

Making use of the plane wave mode representation of the Green's function of equation (9), it is found that

$$\Phi_2(q_1,q_2) = \frac{ik_0^2}{k_z(q_2)} \int d^3r \exp\{i(q_1 - q_2) \cdot \rho + i[k_z(q_2) - \varepsilon k_z(q_1)]z\}\eta(r). \tag{20}$$

20   It is seen that $\Phi_2(q_1,q_2) = \Phi_1(-q_2,-q_1)$, as expected from reciprocity.

- 13 -

2C. Two Probe Mode

Now the case wherein both the source of illumination and the detector of the scattered field are in the near-zone of the scatterer is considered. The source of

5 illumination is taken to be a point source in the $z = 0$ plane with position $r_1 = (\rho_1, 0)$. By way of notation, the case that the scattered field is measured on the $z = z_d$ plane with $z_d = 0$ is referred to as reflection mode detection, and the case that the scattered field is measured on some plane $z = z_d$ with $z_d > 0$ is the transmission mode case. In either mode, the detector position in the $z = z_d$ plane is denoted $r_2 = (\rho_2, z_d)$. This arrangement

10 is shown pictorially in FIG. 3 wherein probe 301 is representative of a source of illumination for sample 105. Probe 302 is the detector for the reflection mode, whereas probe 302 is the detector for the transmission mode.

The incident field is given by equation (10). Consequently, the scattered

15 field is given by

$$U_s(r_1, r_2) = k_0^2 \int d^3 r G(r_2 - r) \eta(r) G(r - r_1). \tag{21}$$

Taking the Fourier transform over both spatial coordinates

$$\Phi_3(q_1, q_2) = \frac{1}{(2\pi)^2} \int d^2 \rho_1 d^2 \rho_2 \exp[i(q_1 \cdot \rho_1 - q_2 \cdot \rho_2)] U_s(\rho_1, 0; \rho_2, z_d), \tag{22}$$

and using the plane wave decomposition of equation (9), the following obtains:

20 $$\Phi_3(q_1, q_2) = -\frac{k_0^2 e^{ik_z(q_2)z_d}}{k_z(q_1)k_z(q_2)} \int d^3 r \exp\{i(q_1 - q_2) \cdot \rho + i[k_z(q_1) - \varepsilon k_z(q_2)]z\} \eta(r). \tag{23}$$

3. NEAR-FIELD INVERSE SCATTERING PROBLEM: SCALAR CASE

In the near-field inverse scattering problem (ISP), the dielectric

susceptibility or scattering function $\eta(r)$ is reconstructed from measurements of the

5   scattered field. It may be observed that equations (16), (20) and (23) are all of similar

form. In order to describe the inverse scattering problem for all three modalities to be

discussed, the following data function is introduced:

$$\Phi(q_1,q_2) = w(q_1,q_2) \int d^3r \exp\{i(q_1-q_2)\cdot\rho + i[k_z(q_1) - \varepsilon k_z(q_2)]\}\eta(r), \tag{24}$$

where

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$$\Phi(q_1,q_2) = \Phi_1(q_1,q_2) \qquad \text{for the illumination mode,} \tag{25a}$$

$$\Phi(q_1,q_2) = \Phi_2(-q_2,-q_1) \qquad \text{for the collection mode,} \tag{25b}$$

$$\Phi(q_1,q_2) = \Phi_3(q_1,q_2) \qquad \text{for the two probe mode.} \tag{25c}$$

Through appropriate choice of the weighting function $w(q_1,q_2)$ all three data functions,

Φ_1, Φ_2, and Φ_3 may be simply related to Φ, that is,

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$$w(q_1,q_2) = \frac{ik_0^2}{k_z(q_1)} \qquad \text{for the illumination mode,} \tag{26a}$$

$$w(q_1,q_2) = \frac{ik_0^2}{k_z(q_2)} \qquad \text{for the collection mode, and} \tag{26b}$$

$$w(q_1,q_2) = \frac{k_0^2 e^{ik_z(q_2)z_d}}{k_z(q_1)k_z(q_2)} \qquad \text{for the two probe mode.} \tag{26c}$$

In all cases, it is assumed that the scattered field can be measured with

20   point-like detection and that the measurement yields both amplitude and phase.

The immediate focus is on the derivation of the singular value decomposition (SVD) of the operator relating Φ to η as defined by integral equation (24). The SVD provides considerable insight into the structure of the forward scattering problem. It also provides a direct technique to construct the pseudo-inverse of the

5 scattering operator. The pseudo-inverse may be used to construct the unique solution to the inverse problem with minimum L^2 norm. In addition to the construction of the minimum norm solution, the SVD presents an obvious procedure by which to regularize the pseudo-inverse through filtering small singular values. This is a significant point for the near-field ISP because of the presence of evanescent waves which exhibit exponential

10 decay. This exponential behavior is a reflection of the ill-posed nature of the problem.

To commence, write equation (24) as

$$\Phi(q_1,q_2) = \int d^3 r K(q_1,q_2;r)\eta(r), \tag{27}$$

where the forward scattering operator $K(q_1,q_2;r)$ is given by

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$$K(q_1,q_2;r) = w(q_1,q_2)\exp\{i(q_1-q_2)\cdot\rho + i[k_z(q_1) - \varepsilon k_z(q_2)]z\}. \tag{28}$$

It is desired to find the SVD of K which is of the form

$$K(q_1,q_2;r) = \int d\sigma\sigma F_\sigma^*(r)G_\sigma(q_1,q_2) \tag{29}$$

where σ is the singular value associated with the singular functions F_σ and G_σ. The

20 singular values and singular functions satisfy the relations

$$\int d^3 r K(q_1,q_2;r)F_\sigma(r) = \sigma G_\sigma(q_1,q_2), \tag{30}$$

and

$$\int d^2q_1 \int d^2q_2 K^*(q_1,q_2;r)G_\sigma(q_1,q_2) = \sigma F_\sigma(r). \tag{31}$$

Equations (30) and (31) are sufficient to define the singular functions and singular values.

It is also possible to derive from these equations the identities

$$K^*K F_\sigma = \sigma^2 F_\sigma, \tag{32}$$

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$$KK^*G_\sigma = \sigma^2 G_\sigma. \tag{33}$$

Here, K is the integral operator whose kernel is $K(q_1,q_2;r)$. The F_σ and G_σ are thus the

eigenfunctions with eigenvalue σ^2 of K^*K and KK^*, respectively.

To obtain the singular values and singular functions, it is worthwhile to

first consider the restricted problem wherein q_2 is fixed and obtain the SVD of

10    $K(q_1,q_2;r)$ which for fixed q_2 is denoted $K_{q_2}(q_1,r)$. Then the following obtains:

$$K_{q_2}(q_1,r) = \int d^2Q \, \sigma_Q^{q_2} f_Q^{q_2 *}(r) g_Q^{q_2}(q_2), \tag{34}$$

$$K_{q_2} f_Q^{q_2} = \sigma_Q^{q_2} g_Q^{q_2}, \tag{35}$$

$$K_{q_2}^* g_Q^{q_2} = \sigma_Q^{q_2} f_Q^{q_2}, \tag{36}$$

where the $f_Q^{q_2}$ and $g_Q^{q_2}$ are the singular functions for fixed q_2 with singular value

15    $\sigma_Q^{q_2}$, labeled by the two dimensional vector Q. The eigenvalue equations then become

$$K_{q_2}^* K_{q_2} f_Q^{q_2} = (\sigma_Q^{q_2})^2 f_Q^{q_2}, \tag{37}$$

$$K_{q_2} K_{q_2}^* g_Q^{q_2} = (\sigma_Q^{q_2})^2 g_Q^{q_2}. \tag{38}$$

By inspection, it is seen that

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$$g_Q^{q_2}(q_2) = \delta(Q + q_2 - q_1), \tag{39}$$

- 17 -

$$f_Q^{q_2}(r) = (\sigma_Q^{q_2})^{-1} w^*(q_2 + Q, q_2) \exp\{-iQ \cdot \rho - i[k_z^*(q_2 + Q) - \varepsilon k_z^*(q_2)]z\}. \tag{40}$$

(Note that an explicit expression for $\sigma_Q^{q_2}$ may be obtained but is not needed.) The

$f_Q^{q_2}$ are orthogonal for fixed q_2,

5
$$\langle f_Q^{q_2} | f_{Q'}^{q_2} \rangle = \delta(Q - Q'). \tag{41}$$

The $f_Q^{q_2}$ are also orthogonal for different q_2, that is,

$$\langle f_Q^{q_2} | f_{Q'}^{q'_2} \rangle = (\sigma_Q^{q_2} \sigma_{Q'}^{q'_2})^{-1} M(q_2, q'_2; Q) \delta(Q - Q'), \tag{42}$$

which defines $M(q_2, q'_2; Q)$.

Returning now to the main problem of finding the SVD of $K(q_1, q_2; r)$,

10   make the ansatz that the G's are constructed from the g_Q^q :

$$G_{QQ'}(q_1, q_2) = C_{Q'}(q_2; Q) g_Q^{q_2}(q_1), \tag{43}$$

where the singular values and the singular functions are labeled with two-dimensional

vectors, Q and Q'. Making use of the relation

$$KK^* G_{QQ'} = \int d^2 q K_q K_q^* G_{QQ'} \tag{44}$$

15   it is found that equations (33) and (38) imply that

$$\int d^2 q' M(q, q'; Q) C_{Q'}(q'; Q) = \sigma^2_{QQ'} C_{Q'}(q; Q). \tag{45}$$

That is, $C_{Q'}(q; Q)$ is an eigenfunction of $M(Q)$ labeled by Q' with eigenvalue $\sigma^2_{QQ'}$.

Since $M(Q)$ is Hermitian, the $C_{Q'}(q; Q)$ may be taken to be orthonormal. It then follows

from equation (31) that

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$$F_{QQ'}(r) = \sigma_{QQ'}^{-1} \int d^2 q C_{Q'}(q; Q) \sigma_Q^q f_Q^q(r). \tag{46}$$

- 18 -

Thus the SVD of $K(q_1, q_2; r)$ is given by

$$K(q_1, q_2; r) = \int d^2Q d^2Q' \sigma_{QQ'} F_{QQ'}^*(r) G_{QQ'}(q_1, q_2). \tag{47}$$

An explicit evaluation of $M(Q)$ shows that $M(q, q'; Q)$ is divergent when

5    $|q|$, $|q'|$, $|Q+q|$, and $|Q+q'|$ are all less than k_0 and also in the case of transmission mode

when $k_z(Q+q) + k_z(Q+q') \geq k_z(q) + k_z(q')$. Of course, this divergence is unphysical.

Any scatterer must be of finite thickness and so, to avoid divergencies, the integration

over r is limited to the region $0 \leq z \leq z_{max}$. Then $M(Q)$ takes the explicit form

$$M(q, q'; Q) = i4\pi^2 w^*(q, Q+q) w(q', Q+q')$$

10
$$\times \frac{1 - \exp\{i(\varepsilon k_z^*(Q+q) + k_z^*(q) - \varepsilon k_z(Q+q') - k_z(q'))z_{max}\}}{\varepsilon k_z^*(Q+q) + k_z^*(q) - \varepsilon k_z(Q+q') - k_z(q')}. \tag{48}$$

In practice, specification of z_{max} acts as a means for including some prior knowledge

about the sample **105** in the model.

15   3A. <u>The Pseudo-inverse</u>

To reconstruct $\eta(r)$ from the data function $\Phi(q_1, q_2)$ it is necessary to first

solve the integral equation $K\eta = \Phi$. Since η and Φ belong to different Hilbert spaces,

the inverse of K as a linear operator is not defined. Instead, a substitute for the solution

is sought which is defined to be a minimizer of $\| K\eta - \Phi \|$. Among all such solutions, it

20   is conventional to choose the one with minimum L^2 norm. This so-called pseudo inverse

solution $\eta^+(r)$ is unique and is given by

$$\eta^+(r) = \int d^2q_1 d^2q_2 K^+(r; q_1, q_2) \Phi(q_1, q_2), \tag{49}$$

where $K^+(r; q_1, q_2)$ is the pseudo-inverse of $K(q_1, q_2; r)$. The pseudo-inverse may be obtained from the SVD of K and is given by the following

$$K^+(r; q_1, q_2) = \int d^2Q d^2Q' \frac{1}{\sigma_{QQ'}} F_{QQ'}(r) G^*_{QQ'}(q_1, q_2). \qquad (50)$$

Using the explicit expressions obtained for the singular functions, K^+ is found to be given by

$$
\begin{aligned}
K^+(r; q_1, q_2) = \int d^2Q \int d^2Q' \int d^2q \delta(Q + q_2 - q_1) \\
\times \sigma_{QQ'}^{-2} C_{Q'}(q; Q) C^*_{Q'}(q_2; Q) w*(q + Q, q) \\
\times \exp\{-iQ \cdot \rho - i(k_z^*(q + Q) - \varepsilon k_z^*(q))z\}.
\end{aligned} \qquad (51)
$$

It may be noted that

$$\int d^2Q' \frac{1}{\sigma_{QQ'}^2} C_{Q'}(q; Q) C^*_{Q'}(q_2; Q) = M^{-1}(q, q'; Q), \qquad (52)$$

where $M^{-1}(q, q'; Q)$ is the qq' matrix element of $M^{-1}(Q)$. Thus

$$
\begin{aligned}
\eta^+(r) = \int d^2q_1 d^2q_2 \int d^2Q d^2q \delta(Q + q_2 - q_1) M^{-1}(q, q'; Q) w^*(q + Q, q) \\
\times \exp\{-iQ \cdot \rho - i(k_z^*(q + Q) - \varepsilon k_z^*(q))z\} \Phi(q_1, q_2),
\end{aligned} \qquad (53)
$$

which is the inversion formula for the near-field ISP.

3B. Regularization

It is known in the art that the singular values for K may be very small and the ISP is ill-posed. Accordingly, the kernel K^+ is highly singular and must be regularized to obtain a stable image reconstruction algorithm. Any of the standard approaches, such as Wiener filtering or the Tikhonov techniques, may be used. For the

SVD-derived pseudo-inverse, these methods result in modification of the singular values via the introduction of a suitable regularizer $R(\sigma)$. More explicitly, equation (50) is can be written as

$$K^+(r;q_1,q_2) = \int d^2Q d^2Q' \frac{1}{\sigma_{QQ'}} R(\sigma_{QQ'}) F_{QQ'}(r) G^*_{QQ'}(q_1,q_2). \quad (54)$$

5   The simplest choice of $R(\sigma)$ consists of simple truncation, which leads to

$$R(\sigma_{QQ'}) = \sigma_{QQ'}^{-1} \theta(\sigma_{QQ'}^{-1} - \sigma_{mn}), \quad (55)$$

for some σ_{mn}. As a variant of this approach, the regularizer may be

$$R(\sigma_{QQ'}) = \sigma_{QQ'}^{-1} \theta(\sigma_{QQ'}^{-1} - \beta \max_Q(\sigma_{QQ'})), \quad (56)$$

where β is the regularization parameter and $\max_Q(\sigma_{QQ'})$ is the largest singular value for

10   a fixed Q. This has the effect of conditioning each of the matrices $M(Q)$ individually. If Tikhonov regularization is used,

$$R(\sigma_{QQ'}) = \frac{\sigma_{QQ'}}{\lambda + \sigma_{QQ'}^2}, \quad (57)$$

where λ is a regularization parameter. This choice leads to smoothing of $\eta^+(r)$ by penalizing functions with large L^2 norm.

15

4. VECTOR SCATTERING THEORY

Now the attention is focused on the vector theory of light. The mathematical treatment of the vector near-field ISP is quite similar to the scalar case; reference is made to the scalar case as needed. Nevertheless, the full vector theory is necessary to consider in depth because the scalar approximation of the scattering of electromagnetic waves breaks down for the case of the dielectric susceptibility $\eta(r)$ varying on subwavelength scales. In addition, the vector approach allows for the incorporation of effects due to polarization.

The attention is on non-magnetic materials, so the focus is only on the electric field E. Consider a monochromatic field of frequency ω. The electric field then satisfies the reduced wave equation

$$\nabla \times \nabla \times E(r) - k_0^2 E(r) = 4\pi k_0^2 \eta(r)E(r), \tag{58}$$

where $\eta(r)$ is the dielectric susceptibility. The field is taken to be composed of two parts,

$$E(r) = E^i(r) + E^s(r), \tag{59}$$

where $E^i(r)$ is the incident field satisfying the homogeneous equation

$$\nabla \times \nabla \times E^i(r) - k_0^2 E^i(r) = 0, \tag{60}$$

and $E^s(r)$ is the scattered field satisfying the equation

$$\nabla \times \nabla \times E^s(r) - k_0^2 E^s(r) = 4\pi k_0^2 \eta(r)E(r). \tag{61}$$

Equation (61) may be recast in integral form

$$E_\alpha^s(r) = k_o^2 \int d^3r' \, G_{\alpha\beta}(r - r') E_\beta(r')\eta(r'), \tag{62}$$

where $G_{\alpha\beta}$ is the electromagnetic free-space Green's tensor satisfying the equation

$$\nabla \times \nabla \times G_{\alpha\beta}(\mathbf{r}) - k_0^2 G_{\alpha\beta}(\mathbf{r}) = 4\pi\delta(\mathbf{r})\delta_{\alpha\beta}. \tag{63}$$

The following notation is used throughout, namely, Greek subscripts indicate vector components and the summation convention applies to repeated indices.

5   Within the accuracy of the first Born approximation, the scattered field is given by

$$E_\alpha^s(\mathbf{r}) = k_o^2 \int d^3r' G_{\alpha\beta}(\mathbf{r}-\mathbf{r}')E_\beta^i(\mathbf{r}')\eta(\mathbf{r}'). \tag{64}$$

The Green's tensor may be obtained from the scalar Green's function by observing that

$$G_{\alpha\beta}(\mathbf{r}) = (\delta_{\alpha\beta} + k_0^{-2}\partial_\alpha\partial_\beta)G(\mathbf{r}). \tag{65}$$

10   Thus it becomes possible to obtain the plane wave decomposition of $G_{\alpha\beta}$ directly by the expression

$$G_{\alpha\beta}(\mathbf{r}) = \frac{i}{2\pi} \int d^2Q k_z(Q)^{-1} T_{\alpha\beta}(Q) \exp\{iQ \cdot \rho + ik_z(Q)|z|\}, \tag{66}$$

where $T_{\alpha\beta}(Q)$ accounts for the polarization of the modes and is given by the expression

$$T_{\alpha\beta}(Q) = \delta_{\alpha\beta} - k_0^{-2}k_\alpha(Q)k_\beta(Q), \tag{67}$$

15   and $k(Q) = (Q, \varepsilon k_z(Q))$.

4A. Illumination Mode

Now turn to the modality considered in Section 2.A in which sample **105** is illuminated by a point source with position $r_1 = (\rho_1, 0)$ which is scanned in the plane

20    $z = 0$. The incident filed is given by

$$E_\alpha^i(\mathbf{r}) = k_0^2 G_{\alpha\beta}(\mathbf{r}-\mathbf{r}')p_\beta \tag{68}$$

where p is the dipole moment of the source of the incident field. Using equation (64), the scattered field is seen to be of the form

$$E_\alpha^s(r) = k_0^4 \int d^3r' \, G_{\alpha\beta}(r-r')\eta(r')G_{\beta\gamma}(r'-r_1)p_\gamma \,. \tag{69}$$

In the far zone of the scatterer, for $|r| \gg |r'|$, the asymptotic form of the Green's function

5   is given by

$$G_{\alpha\beta}(r-r') \sim T_{\alpha\beta}(q)\frac{e^{ikr}}{r}e^{-ik(q)r'}, \tag{70}$$

where equation (12) has been deployed and $k(q) = (q, \varepsilon k_z(q))$ is in the direction of r. It is then seen that the scattered field may be expressed in terms of the scattering amplitude $A_{\alpha\beta}(\rho_1,q)$ as

$$E_\alpha^s(r) \sim k_0^2 A_{\alpha\beta}(\rho_1,q)p_\beta \frac{e^{ikr}}{r}. \tag{71}$$

10

Making use of equations (66), (69), and (70), it is found that

$$A_{\alpha\beta}(\rho_1,q) = k_0^2 T_{\alpha\gamma}(q)\int d^3r' \, G_{\gamma\beta}(r'-r)\exp[-iq\cdot\rho'-i\varepsilon k_z(q)z']\eta(r'). \tag{72}$$

As before, a data function is defined through a Fourier transform of the angular part of the far-zone scattered field,

$$\Phi_\alpha^{(1)}(q_1,q_2) = \frac{1}{2\pi}\int d^2\rho_1 e^{iq_1\cdot\rho_1}A_{\alpha\beta}(\rho_1,q_2)p_\beta. \tag{73}$$

15

Making use of the plane-wave decomposition equation (66), it is found that

$$\Phi_\alpha^{(1)}(q_1,q_2) = \frac{ik_0^2}{k_z(q_1)}T_{\alpha\gamma}(q_2)T_{\gamma\beta}(q_1)p_\beta\int d^3r\exp\{i(q_1-q_2)\cdot\rho+i[k_z(q_1)-\varepsilon k_z(q_2)]z\}\eta(r).$$

$$\tag{74}$$

It may be noted that $\Phi_\alpha^{(1)}$ is identical to Φ_1 except for the polarization factors,

- 24 -

$$\Phi_\alpha^{(1)}(q_1,q_2) = T_{\alpha\gamma}(q_2)T_{\gamma\beta}(q_1)p_\beta\Phi_1(q_1,q_2). \tag{75}$$

4B. Collection Mode

Now consider the modality discussed in Section 2B in which an incident

5   plan wave illuminates sample **105** and the scattered field is measured in the $z = 0$ plane.

The incident field may be expressed as

$$E_\alpha^i(r) = e_\alpha \exp[iq \cdot \rho - i\varepsilon k_z(q)z], \tag{76}$$

where e_α is the polarization incident field. The scattered field, measured in the $z = 0$

plane at the position $r = (\rho_d, 0)$, is given by the expression

10    $$E_\alpha^s(\rho,0;q) = k_0^2\varepsilon_\beta \int d^3r' G_{\alpha\beta}(r-r')\exp[iq \cdot \rho' - i\varepsilon k_z(q)z']\eta(r'). \tag{77}$$

Now define the data function as the Fourier transform of the scattered field

$$\Phi_{\alpha\beta}^{(2)}(q_1,q_2) = \frac{1}{2\pi} \int d^2\rho e^{-iq_2 \cdot \rho} E_\alpha^s(\rho,0;q_1), \tag{78}$$

and use the plane wave decomposition equation (66) to obtain the explicit form

$$\Phi_\alpha^{(2)}(q_1,q_2) = \frac{ik_0^2}{k_z(q_2)}T_{\alpha\beta}(q_2)e_\beta \int d^3r \exp\{i(q_1-q_2) \cdot \rho + i[k_z(q_2) - \varepsilon k_z(q_1)]z\}\eta(r). \tag{79}$$

15   Again it may be seen that $\Phi_\alpha^{(2)}$ and Φ_2 are simply related by the expression

$$\Phi_\alpha^{(2)}(q_1,q_2) = T_{\alpha\beta}(q_2)e_\beta\Phi_2(q_1,q_2). \tag{80}$$

4C. Two Probe Mode

Now the case wherein both the source of illumination and the detector of

20   the scattered field are in the near-zone of the scatterer is considered. The source of

illumination is taken to be a point source in the $z = 0$ plane with position $r_1 = (\rho_1, 0)$. By way of notation, the case that the scattered field measured on the $z = 0$ plane is referred to as the reflection mode, and the case that the scattered field measured on the plane $z = z_d$ with $z_d > 0$ is referred to as the transmission mode case. In either mode, the

5   detector position in the $z = z_d$ plane is denoted $r_2 = (\rho_2, z_d)$. The incident field is given by equation (68). Consequently, the scattered field is given by

$$E_\alpha^s(\rho_1, 0; \rho_2, z_d) = k_0^4 \int d^3 r' G_{\alpha\beta}(r_d - r') G_{\beta\gamma}(r' - r_1) p_\gamma \eta(r'). \qquad (81)$$

Taking the Fourier transform over both spatial coordinates defines a data function

$$\Phi_\alpha^{(3)}(q_1, q_2) = \frac{1}{(2\pi)^2} \int d^2 \rho_1 d^2 \rho_2 \exp[i(q_1 \cdot \rho_1 - q_2 \cdot \rho_2)] E_\alpha^s(\rho_1, 0; \rho_2, z_d). \qquad (82)$$

10   It is then found that the following obtains:

$$\Phi_\alpha^{(3)}(q_1, q_2) = -\frac{k_0^4 e^{i \varepsilon k_z(q_2) z_d}}{k_z(q_1) k_z(q_2)} T_{\alpha\beta}(q_2) T_{\beta\gamma}(q_1) p_\gamma$$
$$\times \int d^3 r \exp\{i(q_1 - q_2) \cdot \rho + i[k_z(q_1) - \varepsilon k_z(q_2)] z\} \eta(r). \qquad (83)$$

15   The data functions $\Phi_\alpha^{(3)}$ and Φ_3 are simply related by

$$\Phi_\alpha^{(3)}(q_1, q_2) = T_{\alpha\beta}(q_2) T_{\beta\gamma}(q_1) p_\gamma \Phi_3(q_1, q_2). \qquad (84)$$

20

5. NEAR-FIELD INVERSE SCATTERING PROBLEM: VECTOR CASE

As in the scalar case, the inverse problem is treated for all three modalities by considering a data function of the form

$$\Phi_\alpha(q_1, q_2) = w_\alpha(q_1, q_2) \int d^3 r \exp\{i(q_1 - q_2) \cdot \rho + i[k_z(q_1) - \varepsilon k_z(q_2)] z\} \eta(r), \qquad (85)$$

25   where

$$\Phi_\alpha(q_1,q_2) = \Phi_\alpha^{(1)}(q_1,q_2), \quad \text{for illumination mode} \tag{86a}$$

$$\Phi_\alpha(q_1,q_2) = \Phi_\alpha^{(2)}(-q_2,-q_1), \quad \text{for collection mode} \tag{86b}$$

$$\Phi_\alpha(q_1,q_2) = \Phi_\alpha^{(3)}(q_1,q_2), \quad \text{for two-probe mode.} \tag{86c}$$

Through appropriate choice of the weighting function $w_\alpha(q_1,q_2)$ all three data functions

5 may be simply related to Φ_α, that is,

$$w_\alpha(q_1,q_2) = -\frac{ik_0^2}{k_z(q_1)} T_{\alpha\gamma}(q_2)T_{\gamma\beta}(q_1)p_\beta, \quad \text{illumination mode} \tag{87a}$$

$$w_\alpha(q_1,q_2) = -\frac{ik_0^2}{k_z(q_2)} T_{\alpha\beta}(q_2)e_\beta, \quad \text{collection mode} \tag{87b}$$

$$w_\alpha(q_1,q_2) = -\frac{k_0^4 e^{i\varepsilon k_z(q_2)zd}}{k_z(q_1)k_z(q_2)} T_{\alpha\beta}(q_2)T_{\beta\gamma}(q_1)p_\gamma, \quad \text{two-probe mode.} \tag{87c}$$

The vector integral equation (85) differs from its scalar counterpart of equation (24) only

10 by a factor associated with polarization. It is clear then that by measuring a fixed

component of the scattered field that the scalar inversion formula of equation (49) may be

used to reconstruct $\eta(r)$. It is advantageous, however, to utilize measurements of all

three components of the scattered field. In this case, the ISP is over-determined and the

SVD of the operator relating Φ_α and η is needed.

15 To obtain the required SVD, begin by writing equation (85) as

$$\Phi_\alpha(q_1,q_2) = \int d^3r K_\alpha(q_1,q_2;r)\eta(r), \tag{88}$$

where the forward scattering operator $K_\alpha(q_1,q_2;r)$ for the vector wave case is given by

$$K_\alpha(q_1,q_2;r) = w_\alpha(q_1,q_2)\exp\{i(q_1-q_2)\cdot\rho + i[k_z(q_1)-\varepsilon k_z(q_2)]z\}. \tag{89}$$

Consider first the restricted problem where q_2 and α are fixed, and obtain

the SVD of the vector operator with components $K_\alpha(q_1, q_2; r)$ which, for fixed q_2 and α,

is denoted $K_{q_2}(q_1, r)$. The SVD is then obtained as follows:

$$K_{q_2\alpha}(q_1, r) = \int d^2 Q \sigma_{Q\alpha}^{q_2} f_{Q\alpha}^{q_2*}(r) g_Q^{q_2}(q_2), \tag{90}$$

5   where the $f_{Q\alpha}^{q_2}$ are the singular functions for fixed q_2 and α with singular values $\sigma_{Q\alpha}^{q_2}$. It

is readily seen that

$$f_{Q\alpha}^{q_2} = (\sigma_{Q\alpha}^{q_2})^{-1} w^*(q_2 + Q, q_2) \exp\{-iQ \cdot \rho - i[k_z^*(q_2 + Q) - \varepsilon k_z^*(q_2)]z\}. \tag{91}$$

As before, an explicit expression for $\sigma_{Q\alpha}^{q_2}$ is not required. The $f_{Q\alpha}^{q_2}$ obey the

orthogonality conditions

10
$$\left\langle f_{Q\alpha}^{q_2} \middle| f_{Q'\alpha}^{q_2} \right\rangle = \delta(Q - Q'), \tag{92}$$

and

$$\left\langle f_{Q\alpha}^{q_2} \middle| f_{Q'\beta}^{q'_2} \right\rangle = (\sigma_{Q\alpha}^{q_2} \sigma_{Q'\beta}^{q'_2})^{-1} M_{\alpha\beta}(q_2, q'_2; Q) \delta(Q - Q'), \tag{93}$$

which defines $M_{\alpha\beta}(q_2, q'_2; Q)$.

15   To find the SVD of the vector operator $K(q_1, q_2; r)$, it is necessary to

determine the eigenfunctions of KK^* which satisfy

$$\sum_\beta K_\alpha K_\beta^* G_{QQ'}^\beta(q_1, q_2) = \sigma_{QQ'}^2 G_{QQ'}^\alpha(q_1, q_2), \tag{94}$$

where the eigenfunctions $G_{QQ'}(q_1, q_2)$ and the singular values $\sigma_{QQ'}$ have been labeled

with two-dimensional vectors Q and Q'. Make the ansatz that the G's are constructed

20   from the g_Q^q:

$$G_{QQ'}^{\alpha}(q_1, q_2) = C_{Q'}^{\alpha}(q_2; Q)g_Q^{q_2}(q_1). \tag{95}$$

Making use of equation (90), it is found that the $C_{Q'}^{\alpha}(q_2; Q)$ are eigenfunctions of

$M_{\alpha\beta}(q, q'; Q)$,

$$\int d^2q' M_{\alpha\beta}(q, q'; Q)C_{Q'}^{\beta}(q'; Q) = \sigma_{QQ'}^2 C_Q^{\alpha}(q; Q), \tag{96}$$

5   with eigenvalues $\sigma_{QQ'}^2$. Next, note that it follows from equation (93) that

$$M_{\alpha\beta}(q, q'; Q) = w_\alpha(q + Q, q)w_\beta(q'+Q, q')A(q, q'; Q), \tag{97}$$

where

$$A(q, q'; Q) = i4\pi^2 \frac{1 - \exp\{i(\varepsilon k_z^*(Q+q) + k_z^*(q) - \varepsilon k_z(Q+q') - k_z(q'))z_{max}\}}{\varepsilon k_z^*(Q+q) + k_z^*(q) - \varepsilon k_z(Q+q') - k_z(q')}. \tag{98}$$

Since the prefactor $w_\alpha(q + Q, q)w_\beta(q'+Q, q')$ of $A(q, q'; Q)$ has the form of a projection

10   operator, it is found that $C_{Q'}^{\alpha}(q; Q)$ may be expressed as

$$C_{Q'}^{\alpha}(q; Q) = \phi_{Q'}(q, Q)\frac{w_\alpha(q + Q, q)}{\Omega(q, Q)}, \tag{99}$$

where

$$\Omega(q, Q) = \left(\sum_\alpha |w_\alpha(q + Q, q)|^2\right)^{1/2}. \tag{100}$$

The $\phi_{Q'}(q; Q)$ are easily seen to be the eigenfunctions of

15    $\tilde{A}(q, q'; Q) = \Omega(q', Q)A(q, q'; Q)\Omega(q, Q)$ with eigenvalues $\sigma_{QQ'}^2$, that is,

$$\int d^2q' \tilde{A}(q, q'; Q)\phi_{Q'}(q'; Q) = \sigma_{QQ'}^2 \phi_{Q'}(q; Q). \tag{101}$$

A second class of eigenfunctions of $M_{\alpha\beta}(q,q';Q)$ may also be seen to exist. However, these eigenfunctions have vanishing singular values and do not contribute to the SVD of K.

5   To complete the development of the SVD, the singular values of $F_{QQ'}(r)$ are required, which as follows from equation (31), are given by

$$F_{QQ'}(r) = \sigma_{QQ'}^{-1} \sum_\alpha K_\alpha^* G_{QQ'}^\alpha \tag{102}$$

$$= \sigma_{QQ'}^{-1} \int d^2q \sum_\alpha C_{Q'}^\alpha(q;Q) \sigma_{Q\alpha}^q f_{Q\alpha}^q(r).$$

Using this result, it is seen that the SVD of $K_\alpha(q_1,q_2;r)$ is given by

10

$$K_\alpha(q_1,q_2;r) = \int d^2Q d^2Q' \sigma_{QQ'} F_{QQ'}^*(r) G_{QQ'}^\alpha(q_1,q_2). \tag{103}$$

The pseudo-inverse of $K_\alpha(q_1,q_2;r)$ may be obtained from the SVD of K_α and is given be the expression

$$K_\alpha^+(r;q_1,q_2) = \int d^2Q d^2Q' \frac{1}{\sigma_{QQ'}} F_{QQ'}(r) G_{QQ'}^{\alpha*}(q_1,q_2). \tag{104}$$

15 Using the expressions previously obtained for the singular functions, K_α^+ is found to be of the form

$$K_\alpha^+(r;q_1,q_2) = \int d^2Q \int d^2Q' \int d^2q \delta(Q+q_2-q_1)$$
$$\times \sigma_{QQ'}^{-2} C_{Q'}^{\alpha*}(q_2;Q) C_{Q'}^\beta(q;Q) w_\beta^*(q+Q,q)$$
$$\times \exp\{-iQ\cdot\rho - i(k_z^*(q+Q) - \varepsilon k_z^*(q))z\}. \tag{105}$$

20   Using the fact that

$$\int d^2 Q' \sigma_{QQ'}^{-2} C_{Q'}^{\alpha *}(q;Q) C_{Q'}^{\beta}(q';Q) = \tilde{A}^{-1}(q,q';Q) \frac{w_{\alpha}^{*}(q+Q,q) w_{\beta}(q'+Q,q')}{\Omega(q,Q)\Omega(q',Q)}, \qquad (106)$$

and the expression for the pseudo-inverse solution

$$\eta^{+}(r) = \int d^2 q_1 d^2 q_2 K_{\alpha}^{+}(r;q_1,q_2)\Phi_{\alpha}(q_1,q_2), \qquad (107)$$

the following obtains:

5
$$\eta^{+}(r) = \int d^2 q_1 d^2 q_2 \int d^2 Q d^2 q \frac{\Omega(q,Q)}{\Omega(q_2,Q)} \delta(Q+q_2-q_1) \tilde{A}^{-1}(q_2,q';Q) w_{\alpha}^{*}(q_2+Q,q_2)$$

$$\times \exp\{-iQ \cdot \rho - i(k_z^{*}(q+Q) - \varepsilon k_z^{*}(q))z\}\Phi(q_1,q_2), \qquad (108)$$

which is the inversion formula for the near-field ISP.

To this point it has been assumed that the scattered field may be measured

10   in its entirety. It may the case that only certain components of the scattered field are

measured. Let $\hat{\xi}$ be a unit vector in the direction in which the scattered field is

measured. The measured quantity will then not be E_{α}^{s} but $\hat{\xi} \cdot E^{s}$. The appropriate data

function to consider for all three modalities in then $\Phi(q_1,q_2) = \hat{\xi}\Phi_{\alpha}(q_1,q_2)$. This

modifies the weight function without otherwise changing the analysis.

15

6A. System

As depicted in high-level block diagram form in FIG. 4, system **400** is a

tomography system for generating an image of an object using measurements of scattered

waves emanating from an object in response to waves illuminating the object. In

20   particular, object **105** is shown as being under investigation. System **400** is composed of:

wave source **420** for probing the object **105**; data acquisition detector **430** for detecting

the scattering data corresponding to the scattered waves from object **105** at one or more

locations proximate to object **105**; position controller **440** for controlling the locations of

detectors **430** and sources **420**; and computer processor **450**, having associated input

5   device **460** (e.g., a keyboard) and output device **470** (e.g., a graphical display terminal).

Computer processor **450** has as its inputs positional information from controller **440** and

the measured scattering data from detector **430**.

Computer **450** stores a computer program which implements the direct

10   reconstruction algorithm; in particular, the stored program processes the measured

scattering data to produce the image of the object or sample under study using a

prescribed mathematical algorithm. The algorithm is, generally, determined with

reference to an integral operator relating the scattering data to the forward scattering

operator (e.g., integral equation (27) wherein the forward scattering operator is

15     $K(q_1, q_2; r)$ or by integral equation (88) wherein the forward scattering operator is

$K_\alpha(q_1, q_2; r)$).

6B. FLOW DIAGRAM

The methodology carried out by the present invention is set forth in high-

20   level flow diagram **500** of FIG. 5 in terms of the illustrative system embodiment shown in

FIG. 4. With reference to FIG. 5, the processing effected by block **510** enables source

420 and data acquisition detector **430** so as to measure the scattering data emanating from

object **105** due to illuminating waves from source **420**. These measurements are passed

to computer processor **450** from data acquisition detector **430** via bus **431**. Next, processing block **520** is invoked to retrieve the pre-computed and stored forward scattering operator. In turn, processing block **530** is operated to execute the reconstruction algorithm set forth with respect to the foregoing equations, thereby

5   determining the scattering potential $\eta(r)$ for the scalar case or dielectric susceptibility $\eta(r)$ for the electromagnetic case. Finally, as depicted by processing block **540**, the reconstructed tomographic image corresponding to $\eta(r)$ is provided to output device **470** in a form determined by the user; device **470** may be, for example, a display monitor or a more sophisticated three-dimensional display device.

10

Although the present invention have been shown and described in detail herein, those skilled in the art can readily devise many other varied embodiments that still incorporate these teachings. Thus, the previous description merely illustrates the

15   principles of the invention. It will thus be appreciated that those with ordinary skill in the art will be able to devise various arrangements which, although not explicitly described or shown herein, embody principles of the invention and are included within its spirit and scope. Furthermore, all examples and conditional language recited herein are principally intended expressly to be only for pedagogical purposes to aid the reader in understanding

20   the principles of the invention and the concepts contributed by the inventor to furthering the art, and are to be construed as being without limitation to such specifically recited examples and conditions. Moreover, all statements herein reciting principles, aspects, and embodiments of the invention, as well as specific examples thereof, are intended to

encompass both structural and functional equivalents thereof. Additionally, it is intended that such equivalents include both currently know equivalents as well as equivalents developed in the future, that is, any elements developed that perform the function, regardless of structure.

5

In addition, it will be appreciated by those with ordinary skill in the art that the block diagrams herein represent conceptual views of illustrative circuitry embodying the principles of the invention.